Title : *ChemAppPy* to model high temperature electrolysis

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There are currently interesting developments of high temperature electrolysis for novel applications such as the direct electrochemical reduction in molten $CaCl_2$-based electrolyte[1], energy storage[2], electrorefining of metals as well as metal production in unconventional electrolytes such as molten oxides[3] and molten sulphides[4]. Experimental work to study high temperature electrolysis is complex and expensive. Time and money can be saved by using numerical simulations to first probe the impact of various operation conditions (such as the electrolyte composition, the temperature and the current density) on the theoretical performance of the targeted electrochemical process. At the moment, classical thermodynamic simulations performed with interface-based software such as *FactSage* cannot directly show the impact of the current density on such energy-intensive processes. Moreover, the user cannot add kinetics consideration (in the form of empirical/semi-empirical models) into these simulations, which also greatly limits the description of the actual reaction mechanisms.

Here, we describe an ongoing project using *ChemAppPy* to estimate the steady state bath composition and product purity at different current density of different electrochemical processes. We discuss methods to estimate the electrochemical potential at the electrodes and how to use kinetic data to increase the accuracy of our simulations. Examples are presented for molten oxides and molten salts electrolysis.

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